N-Ethylglycine 627-01-0 | DTXSID70311675

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 3.22 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

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N-Methylglycine Measured: 3.37 Predicted: 3.48 Image not found

ethylalanine Measured: 4.49 Predicted: 1.99 Image not found

beta-Alanine, N-methyl-Measured: 8.82e-01 Predicted: 1.26

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N-(2-Cyanoethyl)glycine

Measured: 2.11 Predicted: 1.79 Image not found

Methoxyacetic acid Measured: 11.1 Predicted: 7.77